

Time-reversal symmetry breaking surface states in $t - J$ model

Kazuhiro Kuboki^a and Manfred Sigrist^b

^aDepartment of Physics, Kobe University, Kobe 657-8501, Japan

^bYukawa Institute for Theoretical Physics, Kyoto University, Kyoto 606-01, Japan

(Received)

Recently a phenomenological Ginzburg-Landau (GL) theory has been proposed to describe the occurrence of a locally time-reversal symmetry (\mathcal{T}) breaking state near a Josephson junction between unconventional superconductors. In this paper we derive this type of GL free energy microscopically from the $t - J$ model within a slave-boson mean-field approximation. The resulting GL free energy is shown to satisfy the conditions to have a \mathcal{T} -violating surface state. The existence of this junction state may explain some of the recent experiments on High- T_c superconductors.

KEYWORDS: unconventional superconductivity, broken time reversal symmetry

§1. Introduction

The symmetry of the superconducting state in high-temperature superconductors (HTSC) has been a subject of intensive study as an important clue to clarify the mechanism of their superconductivity. The Josephson effect allows us to investigate directly the phase properties of a superconducting order parameter (OP), and thus it is a powerful experimental probe for this study. Many experiments demonstrate that the superconducting OP in these systems has a predominantly $d_{x^2-y^2}$ -wave character, i.e. the OP changes sign under 90° -rotation in the CuO_2 plane^{1,2)}.

In d -wave superconductors interface properties can be qualitatively different from those of conventional superconductors because of the nontrivial angular dependence of their pair wave functions. We have shown that a locally time-reversal symmetry (\mathcal{T}) breaking state can occur near an Josephson junctions between d -wave superconductors and, in general, unconventional superconductors^{3,4,5,6)}. This \mathcal{T} -violating state exists only near the surface and decays exponentially toward the bulk. It has important consequences on Josephson effects. The arguments which led to this conclusion were based on a phenomenological Ginzburg-Landau (GL) theory including several assumptions.^{3,4,5,6,10,11)}

In this paper we derive the GL free energy from the $t - J$ model within a slave-boson mean-field approximation, and demonstrate that it is possible to have a \mathcal{T} -violating surface state. The reason we consider the $t - J$ model is the following. Mean-field (MF) theories of the $t - J$ model based on a slave-boson method predict a superconducting state with a $d_{x^2-y^2}$ -symmetry,^{12,13)} and they may explain the magnetic^{14,15)} as well as the transport¹⁶⁾ properties of HTSC if the gauge fields representing the fluctuations around the MF solutions are properly taken into account. Thus, it is interesting to study whether the $t - J$ model leads to a \mathcal{T} -violating state, in particular, at the Josephson junction.

§2. Mean Field theory and GL expansion of free energy

We consider the $t - J$ model on a square lattice with the Hamiltonian

$$H = -t \sum_{\langle i,j \rangle \sigma} (\tilde{c}_{i,\sigma}^\dagger \tilde{c}_{j,\sigma} + h.c.) + J \sum_{\langle i,j \rangle} \vec{S}_i \cdot \vec{S}_j \quad (2.1)$$

where the summation is taken over nearest-neighbor bonds $\langle i, j \rangle$, and $\tilde{c}_{i\sigma} \equiv c_{i\sigma}(1 - n_{i,-\sigma})$. We use the slave-boson method to enforce the condition of no double occupancy by introducing spinons ($f_{i\sigma}$; fermion) and holons (b_i ; boson) ($\tilde{c}_{i\sigma} = b_i^\dagger f_{i\sigma}$). Then the Hamiltonian is decoupled with the following order parameters (OP)^{12,13)}: (1) the bond OP, $\langle b_j^\dagger b_i \rangle \equiv \chi_B$ and $\langle f_{j\sigma}^\dagger f_{i\sigma} \rangle \equiv \chi_F$ which we assume to be homogeneous for all nearest-neighbor bonds; (2) the OP for the Bose condensation of holons, $\langle b_j b_i \rangle$ ⁷⁾; (3) the singlet RVB OP, $\langle f_{i\uparrow}^\dagger f_{j\downarrow}^\dagger - f_{i\downarrow}^\dagger f_{j\uparrow}^\dagger \rangle \equiv \Delta_{ij}^*$. The superconducting OP is given by the product of the last two, $\langle b_j b_i \rangle \Delta_{ij}^*$. In a slave-boson mean field theory there are four kinds of ordered states in all of which the bond OP are finite: (a) the uniform RVB state where only the bond OPs are finite; b) the spin gap state where the singlet RVB OP is also finite⁸⁾; In this state there is a (pseudo-) gap in the spin, but not in the charge excitations. Hence the name spin gap state; c) the superconducting state where all three OP's listed above are finite; d) the Fermi liquid state⁹⁾. A schematic phase diagram is shown in Fig.1.

In this paper we consider only the optimally and over doped case where $T_{BE} \geq T_{RVB}$, and so the critical temperature for superconductivity, T_c , is given by T_{RVB} . (In other words we do not treat the case where the onset of superconductivity is given by the Bose condensation of holons.) In this case we can take $\chi_B = \delta$, since we always consider the case $T \leq T_{BE}$. Since the superexchange interaction exists only for nearest-neighbor bonds, the $d_{x^2-y^2}$ - and the extended s -wave are natural candidates for the symmetry of the superconducting OP. The for-

mer (latter) is defined by $\Delta_d(i) = (\Delta_{i,i+x} - \Delta_{i,i+y})/2$ ($\Delta_s(i) = (\Delta_{i,i+x} + \Delta_{i,i+y})/2$). Following a standard procedure we expand the free energy with respect to Δ_d and Δ_s .¹⁷⁾ The resulting GL energy is given after taking a continuum limit

$$\begin{aligned}
F = & \int d^3x \left[\sum_{j=d,s} \{ \tilde{a}_j(T) |\Delta_j|^2 + \beta_d |\Delta_j|^4 + K_j |\mathbf{D}\Delta_j|^2 \} \right. \\
& + \gamma_1 |\Delta_d|^2 |\Delta_s|^2 + \frac{1}{2} \gamma_2 (\Delta_d^{*2} \Delta_s^2 + \Delta_d^2 \Delta_s^{*2}) \\
& + \tilde{K} \{ (D_x \Delta_d)^* (D_x \Delta_s) - (D_y \Delta_d)^* (D_y \Delta_s) \\
& \left. + c.c. \} + \frac{1}{8\pi} (\nabla \times \mathbf{A})^2 \right]
\end{aligned} \quad (2.2)$$

where $\vec{D} = \nabla - i(2\pi/\Phi_0)\vec{A}$ with $\Phi_0 (= hc/2e)$ being the standard flux quantum. The coefficients in F are given as

$$\begin{aligned}
\alpha_j &= \frac{3J}{4} \left(1 - \frac{3J}{8N} \sum_k \frac{\tanh(\xi_k/2T)}{\xi_k} \omega_j^2(k) \right) \\
\beta_j &= \left(\frac{3J}{4} \right)^4 \frac{1}{N} \sum_k I(\xi_k) \omega_j^4(k) \\
\gamma &= \left(\frac{3J}{4} \right)^4 \frac{1}{N} \sum_k I(\xi_k) \omega_d^2(k) \omega_s^2(k) \\
K_j &= W_F^2 \frac{9J^2}{32N} \sum_k \frac{f''(\xi_k)}{\xi_k} \sin^2 k_x \omega_j^2(k) \\
\tilde{K} &= W_F^2 \frac{9J^2}{32N} \sum_k \frac{f''(\xi_k)}{\xi_k} \sin^2 k_x \omega_d(k) \omega_s(k)
\end{aligned} \quad (2.3)$$

where $j = d$ or s , $\gamma_1 = 2\gamma$, $\gamma_2 = \gamma/2$, $\omega_d(k) = \cos k_x - \cos k_y$ and $\omega_s(k) = \cos k_x + \cos k_y$. Here

$$\begin{aligned}
I(\xi_k) &= \frac{1}{2\xi_k^2} \left[f'(\xi_k) + \frac{1}{2\xi_k} \tanh\left(\frac{\xi_k}{2T}\right) \right] \\
W_F &= t\delta + \frac{3}{8} J\chi_F
\end{aligned} \quad (2.4)$$

and $f(\xi_k)$ is the Fermi distribution function.

The surface energy at the junction is calculated under the assumption of a specularly reflecting surface. We consider a planar interface parallel to the c -axis as shown in Fig.2. In Fig.2 the left and the right hand side are the same d -wave superconductors described by the $t-J$ model. Here the crystalline a -axis of the left hand side (L) is normal to the interface, while that in the right hand side (R) is taken as a free parameter, denoted as φ ($0 \leq \varphi \leq \pi$). (We can treat an S/D -junction, where the left side is an s -wave superconductor, in a similar way. We consider this case in § 5.) In this configuration the important effects are associated mainly with the OP on the right hand side, so that we will simply represent the left hand side by a single d -wave order parameter Δ_0 only.

The transmission and the reflection of electrons at the interface (I) may be described by the following Hamiltonian,

$$\begin{aligned}
H_I = & \sum_{\sigma} \sum_{k,p} [t_{kp} (f_{k\sigma}^{\dagger(L)} f_{p\sigma}^{(R)} + f_{p\sigma}^{\dagger(R)} f_{k\sigma}^{(L)}) \\
& + r_{kp} (f_{k\sigma}^{\dagger(R)} f_{p\sigma}^{(R)} + f_{p\sigma}^{\dagger(R)} f_{k\sigma}^{(R)})]
\end{aligned} \quad (2.5)$$

where $f_{k\sigma}^{(L)}$ ($f_{k\sigma}^{(R)}$) is the spinon operator for the left (right) side, and the matrix elements for tunneling (t_{kp}) and the reflection (r_{kp}) are taken to be real. Treating H_I in a second-order perturbation theory we get the surface free energy F_I to lowest order in Δ 's,

$$\begin{aligned}
F_I = & \int_I dS \left[\sum_{i,j=\{d,s\}} g_{ij}(\varphi) \Delta_i^* \Delta_j \right. \\
& \left. + \sum_{i=\{d,s\}} t_i(\varphi) (\Delta_0^* \Delta_i + \Delta_0 \Delta_i^*) \right].
\end{aligned} \quad (2.6)$$

The first term originates from the reflection of the Cooper pairs at the interface and the second term represents the coupling between the two sides ($g_{ij} = g_{ji}$). For the D/D -junction composed of the same superconductors, the coefficients in eq.(2.6) are given as

$$\begin{aligned}
t_d &= \left(\frac{3J}{4} \right)^2 \sum_{kp} t_{kp}^2 J_1(\xi_k, \xi_p) \omega_d(k) \omega_d(p) \\
t_s &= \left(\frac{3J}{4} \right)^2 \sum_{kp} t_{kp}^2 J_1(\xi_k, \xi_p) \omega_d(k) \omega_s(p) \\
g_d &= \left(\frac{3J}{4} \right)^2 \sum_{kp} [r_{kp}^2 J_1(\xi_k, \xi_p) \omega_d(k) \omega_d(p) \\
&+ (r_{kp}^2 + t_{kp}^2) J_2(\xi_k, \xi_p) \omega_d(k)^2] \\
g_s &= \left(\frac{3J}{4} \right)^2 \sum_{kp} [r_{kp}^2 J_1(\xi_k, \xi_p) \omega_s(k) \omega_s(p) \\
&+ (r_{kp}^2 + t_{kp}^2) J_2(\xi_k, \xi_p) \omega_s(k)^2] \\
g_{ds} &= \left(\frac{3J}{4} \right)^2 \sum_{kp} [r_{kp}^2 J_1(\xi_k, \xi_p) \omega_s(k) \omega_d(p) \\
&+ (r_{kp}^2 + t_{kp}^2) J_2(\xi_k, \xi_p) \omega_d(k) \omega_s(k)]
\end{aligned} \quad (2.7)$$

with

$$\begin{aligned}
J_1(\xi_k, \xi_p) &= \frac{1}{\xi_k^2 - \xi_p^2} \left(\frac{\tanh(\frac{\xi_k}{2T})}{2\xi_k} - \frac{\tanh(\frac{\xi_p}{2T})}{2\xi_p} \right) \\
J_2(\xi_k, \xi_p) &= \frac{2\xi_k}{\xi_k - \xi_p} I(\xi_k) \\
&+ \frac{\xi_p}{(\xi_k + \xi_p)(\xi_k - \xi_p)^2} \left(\frac{\tanh(\frac{\xi_k}{2T})}{\xi_k} - \frac{\tanh(\frac{\xi_p}{2T})}{\xi_p} \right).
\end{aligned} \quad (2.8)$$

The J_1 terms represent the usual tunneling and the reflection processes of a Cooper pair. On the other hand, the J_2 terms give different types of reflection processes where one of the particle consisting of a Cooper is reflected at the interface, while the other one tunnels to the opposite side (see in the Appendix for the derivation of the surface terms and the interpretation of J_2).

Here we follow the method of Ref.^{18,19)} in taking the angular dependences of t_{kp} and r_{kp} , which are consistent

with the assumption of the specularly reflecting surface,

$$\begin{aligned} t_{kp}^2 &= \tilde{t}^2 \delta(k_{\parallel} - p_{\parallel}) \delta(k_{\perp} - p_{\perp}) \frac{v_{\perp}(p)}{v(p)} \theta(v_{\perp}(p)) \\ r_{kp}^2 &= \tilde{r}^2 \delta(k_{\parallel} - p_{\parallel}) \delta(k_{\perp} + p_{\perp}) \frac{v_{\perp}(p)}{v(p)} \theta(v_{\perp}(p)) \end{aligned} \quad (2.9)$$

where θ is the step function. It should be noted here that if the angular dependences of the tunneling matrix elements were omitted, the coupling between two superconductors should vanish, and thus it would lead to unphysical results.

§3. Relation to Phenomenological Theory

Now let us briefly summarize the content of the phenomenological theory of Ref.4 to describe a \mathcal{T} -violating surface state. The properties of the bulk system are described by the free energy F . We assume that only a d -wave OP is present in the bulk system, and the coupling between Δ_d and Δ_s is repulsive, if the latter were present. Namely, a_d is negative below a critical temperature, while $a_s > 0$ for all T , and $\gamma_1 - \gamma_2 > 0$ and $\gamma_2 > 0$. An important point here is that positive γ_2 favors the relative phase between Δ_d and Δ_s , denoted as ϕ_{ds} , to be $\pm\pi/2$, i.e., the system would break \mathcal{T} if both d and s -components coexist. We expect $\gamma_2 > 0$ for the following reason. The complex combination $d \pm is$, resulting from $\gamma_2 > 0$, would open a complete gap in the excitation spectrum, such that the system would gain more condensation energy. If $\phi_{ds} = 0$ or π ($(d \pm s)$ -state), the nodes remain though their locations are shifted, and the gain of the condensation energy would be smaller.

The interface properties are described by F_I . In the presence of an interface, Δ_s can be induced by the reflection of Cooper pairs and by the proximity effect from Δ_0 in (L) . These processes are possible because of the lowering of the symmetry (translational and point-group) in the presence of the interface. In usual cases ϕ_{ds} is determined by the bilinear coupling terms in F_I which induces the finite Δ_s . On the other hand, the γ_2 term favoring $\phi_{ds} = \pm\pi/2$ is biquadratic and it would not be dominant in the sense of GL theory. Then ϕ_{ds} takes a value 0 or π depending on the sign of t_d , t_s and g_{ds} . There is no \mathcal{T} -breaking in this case. Under certain conditions, however, a different relative phase is favored leading to a state which breaks \mathcal{T} . In Ref.4 it was argued based on the symmetry consideration that t_d and g_{ds} should vanish at $\theta = \pi/4$ and are small for θ close to $\pi/4$, while t_s remains always finite. Then, for $\theta \sim \pi/4$ ϕ_{ds} is determined by γ_2 , and, thus, it is possible to have a locally \mathcal{T} -violating state near the interface.

We numerically calculate coefficients in F and F_I as functions of the doping rate δ and the temperature T . We take $t/J = 3$ throughout in this paper. First we solve the self-consistency equations for the uniform RVB state (the state where only χ_F and $\chi_B = \delta$ are finite), to get χ_F and the chemical potential, λ_F . By using them we calculate the coefficients in F and F_I . For the doping rate where the superconductivity is observed in real systems, i.e., $0 < \delta < 0.3$, only α_d can be negative and all other coefficients of F are positive definite²⁰). This im-

plies that we deal with a single d -wave component. We find indeed a positive γ_2 which favors the phase difference $\phi_{ds} = \pm\pi/2$. Hence, the above results are consistent with the assumptions of the previous purely phenomenological theory.

Next we consider the interface terms F_I . By taking the angular dependences of t_{kp} and r_{kp} as in eq.(2.9), we get the coefficients in F_I as functions of φ , i.e., the angle between the interface and the crystal a -axis of the right hand side. We can explicitly examine the following properties using the expressions of t_i and g_{ij} ($i, j = d, s$):

$$\begin{aligned} t_s(\varphi \pm \pi/2) &= t_s(\varphi), \quad t_d(\varphi \pm \pi/2) = -t_d(\varphi) \\ t_s(\varphi \pm \pi) &= t_s(\varphi), \quad t_d(\varphi \pm \pi) = t_d(\varphi) \\ t_s(-\varphi) &= t_s(\varphi), \quad t_d(-\varphi) = t_d(\varphi) \end{aligned} \quad (3.1)$$

and

$$\begin{aligned} g_{ii}(\varphi \pm \pi/2) &= g_{ii}(\varphi), \quad g_{ds}(\varphi \pm \pi/2) = -g_{ds}(\varphi) \\ g_{ii}(\varphi \pm \pi) &= g_{ii}(\varphi), \quad g_{ds}(\varphi \pm \pi) = g_{ds}(\varphi) \\ g_{ii}(-\varphi) &= g_{ii}(\varphi), \quad g_{ds}(-\varphi) = g_{ds}(\varphi) \end{aligned} \quad (3.2)$$

where $i = d, s$. We have calculated t_i and g_{ij} numerically, as shown in Fig. 3, with a choice of parameters $\delta = 0.15$ and $T = 0.8T_c$ ($T_c \sim 0.108J$). The important point here is that t_s does not vanish for any value of φ . This property is robust for any doping δ and temperature T . Another point is that $|t_s|$ is much smaller than $|t_d|$ except very near $\varphi = \pi/4$. This can be explained as follows. The integrand in the expression of t_s has a factor $(\cos k_x + \cos k_y)$, while that of t_d has $(\cos k_x - \cos k_y)^2$. Since we are treating the square lattice system, the factor $(\cos k_x + \cos k_y)$ is small everywhere on the Fermi surface, for the doping rate as small as $\delta = 0.15$, while the factor $(\cos k_x - \cos k_y)^2$ can be large there. Hence $|t_d|$ can be much larger than $|t_s|$. (For $\varphi = \pi/4$, t_d has to vanish by symmetry. Then $|t_s|$ can be larger than $|t_d|$ if φ is close enough to $\pi/4$.)

§4. \mathcal{T} -breaking state and Surface Current

In this section we analyze the appearance of the \mathcal{T} -breaking state. For this purpose we minimize the total free energy, $F_{tot} = F + F_I$, with respect to the OP, Δ_s and Δ_d , and the vector potential \vec{A} . We use a coordinate system (\tilde{x}, \tilde{y}) , with \tilde{x} (\tilde{y}) being perpendicular (parallel) to the interface. Under the transformation from (x, y) to (\tilde{x}, \tilde{y}) , only \tilde{K} terms are changed, and it transforms to

$$\begin{aligned} \tilde{K} [\cos 2\varphi \{ (D_{\tilde{x}} \Delta_d) (D_{\tilde{x}} \Delta_s)^* - (D_{\tilde{y}} \Delta_d) (D_{\tilde{y}} \Delta_s)^* \} \\ + \sin 2\varphi \{ (D_{\tilde{x}} \Delta_d) (D_{\tilde{y}} \Delta_s)^* + (D_{\tilde{y}} \Delta_d) (D_{\tilde{x}} \Delta_s)^* \}]. \end{aligned} \quad (4.1)$$

Since there is no spatial variation of the OP along \tilde{y} -direction, the GL equations are formally written as

$$\frac{\partial F}{\partial \Delta_i(\tilde{x})} = \partial_{\tilde{x}} \frac{\partial F}{\partial (\partial_{\tilde{x}} \Delta_i(\tilde{x}))} \quad (i = d, s) \quad (4.2)$$

and

$$\begin{aligned} J_{\tilde{x}} &\equiv -\frac{\partial F}{\partial A_{\tilde{x}}} = 0, \\ J_{\tilde{y}} &\equiv -\frac{\partial F}{\partial A_{\tilde{y}}} = -\frac{1}{4\pi} \partial_{\tilde{x}} B \end{aligned} \quad (4.3)$$

where $B = \nabla_{\tilde{x}} A_{\tilde{y}} - \nabla_{\tilde{y}} A_{\tilde{x}}$ and $A_{\tilde{x}} = A_x \cos \varphi - A_y \sin \varphi$, $A_{\tilde{y}} = A_x \sin \varphi + A_y \cos \varphi$. The boundary conditions at the interface are

$$\left(\frac{\partial F}{\partial (\nabla_{\tilde{x}} \Delta_i(\tilde{x}))} + \frac{\partial F_I}{\partial \Delta_i(\tilde{x})} \right) \Big|_{\tilde{x}=0} = 0 \quad (i = d, s) \quad (4.4)$$

and

$$B(\tilde{x} = 0) = 0. \quad (4.5)$$

Now we analyze the instability to a \mathcal{T} -violating state at the temperature T^* . We consider a junctions as described in Fig.2, and assume that on both sides the superconductors have the same properties, in particular, the same T_{cd} . At $T = T_c$, Δ_d and Δ_0 (d -wave) get finite, and Δ_s is induced simultaneously near the interface due to the t_s and g_{ds} term. For $\varphi = \pi/4$, t_d and g_{ds} vanish, so only the γ_2 term determines the relative phase ϕ_{ds} . Since $\gamma_2 (> 0)$ favors $\phi_{ds} = \pm\pi/2$, \mathcal{T} -breaking occurs. Thus for $\varphi = \pi/4$, we have $T^* = T_c$, namely, \mathcal{T} -violation should occur at T_c , the bulk superconducting transition temperature, irrespective of any other details.

Numerical calculation for the GL equations confirms this argument. We have solved GL equations (4.2) and (4.3) under the boundary conditions, eq. (4.4) and (4.5). In Fig.4 we show the spatial dependences of Δ_d , Δ_s and ϕ_{ds} for $\delta = 0.15$, i.e., so-called optimum doping. The results for other values of δ is qualitatively the same. For $\varphi = \pi/4$, ϕ_{ds} always takes a value $\pi/2$ or $-\pi/2$, once T becomes lower than T_c . As φ moves away from $\pi/4$, t_d and g_{ds} become finite and compete with γ_2 , which favors \mathcal{T} -breaking states. Since t_d grows very rapidly as φ moves away from $\pi/4$, T^* drastically decreases as a function of $|\varphi - \pi/4|$ (see Fig.5.).

However, we should note here that at very low temperature the region of \mathcal{T} -violation can be much larger because of the following reason. If T is lower than T_{cs} , there is a chance to have finite Δ_s without using tunneling terms. In this case both t_d and t_s can be smaller than γ_2 , with keeping Δ_s finite²¹⁾. Unfortunately T_{cs} derived from the $t - J$ model is quite low (of the order of $10^{-3} J$ corresponding to $T_{cs}/T_{cd} \sim 10^{-2}$), so the region $T < T_{cs}$ is not accessible by the GL theory.

It has been shown that in a \mathcal{T} -breaking state the surface current along the interface can flow.^{10, 22, 23)} The condition for the minimum free energy requires the vanishing of the current normal to the junction (i.e., the first equation of (4.3)). This condition in turn leads to a finite current along the junction which induces a magnetic field. In Fig.6 the spatial distributions of the surface current and the magnetic field are shown. The extension of the current and the magnetic field are of the order of the penetration depth λ . Note that no net current is present, i.e. the integrated current vanishes²⁴⁾,

$$\int_0^L d\tilde{x} J_{\tilde{y}}(\tilde{x}) = \frac{1}{4\pi} [B(\tilde{x} = 0) - B(\tilde{x} = L)] = 0 \quad (4.6)$$

where L is the length of the system ($L \gg \lambda$), and we have used eq.(4.5).

§5. Case of S/D -junctions

So far we have considered only D/D -junctions, where both sides are the same d -wave superconductors. The S/D -junction (where the left side is replaced by a different superconductor with isotropic s -wave symmetry) can be treated similarly.

We consider a conventional superconductor for the left side of the junction. We take the band width, the chemical potential and the magnitude of the order parameter in (L) to be the same as in (R) for simplicity. Our aim here is to compare the qualitative features of D/D - and S/D -junctions, but not the quantitative comparison.

The surface GL energy can be calculated in a similar way as in § 2. The modified expressions are simply given by the replacement

$$\omega_d(k) \rightarrow 1 \quad (5.1)$$

in eq.(2.7) for t_d and t_s . For the S/D -junction $|t_s|$ is larger than $|t_d|$ (for φ not so far apart from $\pi/4$), in contrast to the case of D/D -junctions. (Fig. 7) However, the value of $|t_s|$ in this case is much smaller than that of $|t_d|$ for D/D -junction. This is due to the same reason as we have $|t_d| \gg |t_s|$ for the D/D -junction: the factor $(\cos k_x + \cos k_y)$ is always small on the Fermi surface, and so $|t_s|$ is reduced even if the OPs of both sides have s -wave symmetry.

The phase diagram of surface states for S/D -junction is shown as a solid line in Fig.5. In Fig.8 the φ -dependence of the relative phases between Δ_d and Δ_s (Δ_0), ϕ_{ds} (ϕ_0) is also shown. We find that in the phase diagram the region of \mathcal{T} -breaking states is larger than for the D/D -junction. This is the case even when we assume a rather small value of $|\Delta_0|/|\Delta_d^{bulk}|$. In S/D -junction $|\Delta_s|$ can be sizable due to large $|t_s|$, and then the γ_2 -term (fourth order) which favors \mathcal{T} -violating states can compete with the second order terms (t_d and g_{ds}) even when φ is not so close to $\pi/4$. In the case of D/D -junction, however, t_d and g_{ds} become dominant once φ moves away from $\pi/4$, leading to a very limited region of \mathcal{T} -violating states.

§6. Conclusions

We have discussed the S/D - and D/D -interface states using a GL-formulation derived from the slave-boson mean-field approximation for the $t - J$ model. The \mathcal{T} -violating interface state was found in both cases for certain orientations in agreement with previous phenomenological studies.

In addition we found that the \mathcal{T} -violating state is more likely to occur on an S/D - than on a D/D -interface. This distinction is mainly due to the fact that the Josephson coupling to a d -wave superconductor is generally weaker, because of the angular phase structure of the pair wave function which leads to destructive interference in the tunneling. Furthermore, the shape of the Fermi surface plays an important role, in particular, for the extended S -wave state.

Within the GL theory the range of angles φ where the \mathcal{T} -violating state can appear is rather small for the D/D -junction. However, it should be noted that for tem-

peratures below T_{cs} this region in the phase diagram could extend to a wider range. Obviously, the GL formulation does not allow us to access this temperature region. In our approach the ratio T_{cs}/T_{cd} is of the order 10^{-2} so that temperatures below T_{cs} are definitely far away from the range of validity of a GL theory. The low-temperature region can only be treated by methods based on Bogolyubov-de Gennes equations or quasiclassical theory which are considerably more complicated if one intends to include more realistic microscopic details.

Previously a series of phenomena were discussed, in connection with broken time reversal symmetry on interfaces. A first example are flux lines on the interface which do enclose neither integer nor half-integer multiples of the standard flux quanta, but some intermediate fractional fluxes^{3, 4, 25}. Although the observation of fractional flux by Kirtley et al.²⁶ is entirely compatible with our discussion here, it is not clear whether the data could not be explained in an alternative way. The main problem for this kind of experiments lies in the requirement of comparatively long homogeneous interfaces, a condition hard to satisfy with present technology. On the other hand, it was also discussed that phase slip effects on short interfaces could be used as a test²⁷. So far no experimental data are available for this type of effect. Finally an important aspect of the \mathcal{T} -violating state is the presence of spontaneous currents. Their magnitude is small, however, and together with screening effects they would not lead to a net magnetization. Thus only a very sensitive probe with high spatial resolution, smaller or of order London penetration depth, would be sufficient to observe this effect. Until now the only method which has successfully observed the small magnetic fields induced by a \mathcal{T} -violating state are muon spin rotation measurements in zero external field²⁸.

It is important to notice, however, that also surfaces of d-wave superconductors can yield states with locally broken time reversal symmetry. Recent experiments indicate that this type of state might be realized at low temperatures on YBCO surfaces with [110]-orientation²⁹. The evidence is given by the splitting of the zero-bias anomaly in the IV -characteristics as discussed by Fogelström et al.³⁰. Clearly similar effects due to the rearrangement of quasiparticle states are also expected in \mathcal{T} -violating interfaces as discussed by Huck et al. and could possibly be tested by spectroscopy with a scanning tunneling microscope³¹.

Acknowledgment

We are grateful to P.A Lee, T.M. Rice, H. Fukuyama and M. Ogata for stimulating discussions. K.K was supported by Grant-in Aid for Scientific Research on Priority Areas "Anomalous metallic state near the Mott transition" from the Ministry of Education, Science and Culture of Japan.

Appendix: Derivation of surface terms

The surface free energy F_I in §2 is derived in the following way. We describe the transmission and the reflection of electrons at the interface by the Hamiltonian H_I in eq.(5). Then the total Hamiltonian is given

by $H + H_I$. Second order perturbation theory gives the excess energy due to H_I :

$$\Delta F = -\frac{1}{2} \int_0^\beta d\tau \langle T_\tau H_I(\tau) H_I(0) \rangle_0 \quad (\text{A.1})$$

where $\langle \cdots \rangle_0$ denotes the average with respect to H . We substitute eq.(5) into this expression and decouple it in terms of Green's functions of spinons for both sides

$$\begin{aligned} \Delta F &= \Delta F_1 + \Delta F_2 \\ \Delta F_1 &= - \sum_{kp} T \sum_{\epsilon_n} [t_{kp}^2 \{ G_{21}^L(p, i\epsilon_n) G_{12}^R(k, i\epsilon_n) \\ &\quad + G_{12}^L(p, i\epsilon_n) G_{21}^R(k, i\epsilon_n) \} + r_{kp}^2 G_{21}^R(p, i\epsilon_n) G_{12}^R(k, i\epsilon_n)] \\ \Delta F_2 &= - \sum_{kp} T \sum_{\epsilon_n} [t_{kp}^2 \{ G_{11}^L(p, i\epsilon_n) G_{11}^R(k, i\epsilon_n) \\ &\quad + G_{22}^L(p, i\epsilon_n) G_{22}^R(k, i\epsilon_n) \} \\ &\quad + \frac{1}{2} r_{kp}^2 \{ G_{11}^R(p, i\epsilon_n) G_{11}^R(k, i\epsilon_n) + G_{22}^R(p, i\epsilon_n) G_{22}^R(k, i\epsilon_n) \}] \end{aligned} \quad (\text{A.2})$$

where the Green's functions are defined by

$$\begin{aligned} G_{11}^A(k, i\epsilon_n) &= -\frac{i\epsilon_n + \xi_k}{\epsilon_n^2 + \xi_k^2 + |\Delta_k^A|^2} \\ G_{22}^A(k, i\epsilon_n) &= -\frac{i\epsilon_n - \xi_k}{\epsilon_n^2 + \xi_k^2 + |\Delta_k^A|^2} \\ G_{12}^A(k, i\epsilon_n) &= -\frac{\Delta_k^A}{\epsilon_n^2 + \xi_k^2 + |\Delta_k^A|^2} \\ G_{21}^A(k, i\epsilon_n) &= G_{12}^A(k, i\epsilon_n)^* \end{aligned} \quad (\text{A.3})$$

with $A = R$ or L , $\epsilon_n = \pi T(2n + 1)$, $\Delta_k^R = (3J/4)(\Delta_d \omega_d(k) + \Delta_s \omega_s(k))$ and $\Delta_k^L = (3J/4)\Delta_0 \omega_d(k)$. Now we extract the lowest order ($O(\Delta^2)$) terms. In ΔF_1 there are terms of the form $\Delta^L \Delta^R$ and $\Delta^R \Delta^R$ in the numerator. The former results in the t_i -terms, and the latter leads to the part of the g_{ij} -terms. We can also obtain the $O(\Delta^2)$ terms from the denominators of G_{11} and G_{22} in ΔF_2 . These terms are usually discarded in the discussion of the Josephson effect, since it does not depend on the phase difference of Δ 's if both sides of the superconductors have only one component of the order parameter. In the present case, however, this term depends on the phase difference of Δ_d and Δ_s , and thus it is equally important as the one from ΔF_1 . Neglecting terms independent of Δ , we perform the ϵ_n -summation in eq.(A2) to get the following expressions

$$\begin{aligned} \Delta F_1 &= - \sum_{kp} J_1(\xi_k, \xi_p) [t_{kp}^2 \{ (\Delta_p^L)^* \Delta_k^R + \Delta_p^L (\Delta_k^R)^* \} \\ &\quad + r_{kp}^2 (\Delta_p^R)^* \Delta_k^R] \\ \Delta F_2 &= \sum_{kp} J_2(\xi_k, \xi_p) (t_{kp}^2 + r_{kp}^2) |\Delta_p^R|^2 \end{aligned} \quad (\text{A.4})$$

The expressions for t_i and g_{ij} (eq.(7) in §2) can be obtained from eq.(A4). For example, g_d is given by the coefficients of $|\Delta_d|^2$ in $\Delta F = \Delta F_1 + \Delta F_2$.

The meaning of the J_2 -terms is now obvious. Since we got these terms by picking up $|\Delta_p^R|^2$ in G_{11}^R and G_{22}^R (diagonal components of the Green's functions), only one particle is transferred from (L) to (R) (or (R) to (L)) in this process. This means that one of the electrons consisting of a Cooper pair tunnels to the other side, while the other one is reflected when the Cooper is scattered at the interface. Hence the process including t_{kp} (tunneling matrix element) can lead to the suppression (g_d and g_s) and the interference (g_{ds}) of the superconducting order parameters.

- 1) D.A. Wollman *et al.*, Phys. Rev. Lett. **71**, 2134 (1993) ; D. Brawner and H.R. Ott, Phys. Rev. B **50**, 6530 (1994); A. Mathai *et al.*, Phys. Rev. Lett. **74**, 4523 (1995) ; C.C. Tsuei *et al.*, Phys. Rev. Lett. **73**, 593 (1994) ; I. Iguchi and Z. Wen, Phys. Rev. B **49**, 12388 (1994).
- 2) M. Sigrist and T.M. Rice, J. Phys. Soc. Jpn. **61**, 4283 (1992).
- 3) M. Sigrist, D. Bailey and R. Laughlin, Phys. Rev. Lett. **74**, 3249 (1995).
- 4) K. Kuboki and M. Sigrist, J. Phys. Soc. Jpn., **65** 361 (1996) ; Czech. J. of Phys. **46**-Suppl., 1039-1040 (1996).
- 5) M. Sigrist, K. Kuboki, P.A. Lee, A.J. Millis and T.M. Rice, Phys. Rev. **B53**, 2835 (1996).
- 6) M. Sigrist, K. Kuboki, A.B. Kuklov, D.B. Bailey and R.B. Laughlin, Czech. J. of Phys. **46**-Suppl., 3159-3164 (1996).
- 7) In 2D Bose condensation in a usual sense would not occur. However, there exists a crossover temperature, T_{BE} , below which bosons are almost condensed to the lowest energy state. The true condensation occurs with a small three dimensionality which is always present in real systems.
- 8) In this state there is a (pseudo-) gap in the spin, but not in the charge excitations.
- 9) In this theory the Fermi liquid state is represented as an ordered state where holons are Bose condensed. In this case the system has only fermionic degrees of freedom (spinons), and thus represent a Fermi liquid state.
- 10) A similar result was obtained from quasiclassical theory in M. Matsumoto and H. Shiba, J. Phys. Soc. Jpn., **64**, 3384 (1995).
- 11) S. Yip, Phys. Rev. **B52**, 3087 (1995).
- 12) Y. Suzumura, Y. Hasegawa and H. Fukuyama, J. Phys. Soc. Jpn., **57**, 580 (1988).
- 13) G. Kotliar and J. Liu, Phys. Rev., **B38**, 5142 (1988).
- 14) T. Tanamoto, K. Kuboki and H. Fukuyama, J. Phys. Soc. Jpn., **60**, 3072 (1991).
- 15) H. Fukuyama, H. Kohno, B. Normand and T. Tanamoto, J. Low Temp. Phys., **99**, 429 (1995).
- 16) N. Nagaosa and P.A. Lee, Phys. Rev. Lett., **64** (1990) 2450; P.A. Lee and N. Nagaosa, Phys. Rev. **B46**, 5621 (1992).
- 17) For a review see M. Sigrist and K. Ueda, Rev. Mod. Phys., **63**, 239 (1991).
- 18) C. Bruder, A. van Otterlo and G.T. Zimanyi, Phys. Rev. **B51**, 12904 (1995).
- 19) Yu.S. Barash, A.V. Galaktionov and A.D. Zaikin, Phys. Rev. **B52**, 665 (1995).
- 20) At very low temperature, of the order of $10^{-3}J$, α_s can be negative. However, the GL theory could not be applied to such a low T .
- 21) Y. Tanuma, Y. Tanaka, M. Ogata and S. Kashiwaya, to appear in J. Phys. Soc. Jpn.: In this paper the surface state of the $t-J$ model (surface is faced to vacuum) is studied at $T=0$, using Bogoliubov - de Gennes method based on a Gutzwiller approximation. The \mathcal{T} -breaking state is found at $\varphi = \pi/4$, but not for $\varphi = 0$.
- 22) G.E. Volovik and L.P. Gorkov, Zh. EKsp. Teor. Fiz. **88**, 1412 (1985) [Sov. Phys. JETP **61**, 843 (1985)].

- 23) M. Sigrist, T.M. Rice and K. Ueda, Phys. Rev. Lett., **63**, 1727 (1989).
- 24) Y. Ohashi and T. Momoi, J. Phys. Soc. Jpn, **65**, 3254 (1996).
- 25) M. Sigrist and Y.B. Kim, J. Phys. Soc. Jpn. **63**, 4314 (1994).
- 26) J.R. Kirtley *et al.*, Phys. Rev. **B51**, 12057 (1995).
- 27) A.B. Kuklov and M. Sigrist, Int. J. Mod. Phys. **11**, 1113 (1997).
- 28) A. Amato, Rev. Mod. Phys. **69**, 1119 (1997).
- 29) M. Covington, M. Aprili, E. Paraoanu, L.H. Greene, F. Xu, J. Zhu and C.A. Mirkin, Phys. Rev. Lett. **79**, 277 (1997).
- 30) M. Fogelström, D. Rainer and J.A. Sauls, Phys. Rev. Lett. **79**, 281 (1997).
- 31) A. Huck, A. van Otterlo and M. Sigrist, Phys. Rev. **B56**, 14163 (1997).

Fig. 1. Schematic phase diagram of the $t-J$ model within a slave-boson mean-field approximation. T_χ , T_{RVB} and T_{BE} are the transition temperature for the bond order, singlet RVB order and the Bose condensation, respectively.

Fig. 2. Interface between d -wave superconductors. The lines on both sides indicate the crystalline a -axis (the c -axis points out of the plane).

Fig. 3. Numerical results of the coefficients in F_I for D/D -junction: (a) t_d and (b) g_{ij} ($i, j = d, s$). Here $\delta = 0.15$, $T = 0.8T_c$, $\tilde{t}^2 = 8.0$ and $\tilde{r}^2 = 0.2$.

Fig. 4 Spatial variation of the order parameters and their relative phase. Here $\delta = 0.15$, $\tilde{t}^2 = 8.0$ and $\tilde{r}^2 = 0.2$ and $\varphi = \pi/4$.

Fig. 5. Phase diagram of surface states in the plane of T and φ . Here $\delta = 0.15$, $\tilde{t}^2 = 8.0$ and $\tilde{r}^2 = 0.2$. The line is for the D/D (S/D)-junction. (The \mathcal{T} -breaking region for D/D -junction is invisible in this scale.)

Fig. 6. Distributions of the surface current J_y (A/cm²) and the local magnetic field B (G). Here $\delta = 0.15$, $T = 0.8T_c$, $\tilde{t}^2 = 8.0$, $\tilde{r}^2 = 0.2$ and $\varphi = \pi/4$.

Fig.7 Numerical results of the coefficients in F_I for S/D -junction. Here $\delta = 0.15$, $T = 0.8T_c$, $\tilde{t}^2 = 8.0$ and $\tilde{r}^2 = 0.2$.

Fig.8 The relative phases between Δ_d and Δ_s (Δ_0), ϕ_{ds} (ϕ_0) as a function of φ .

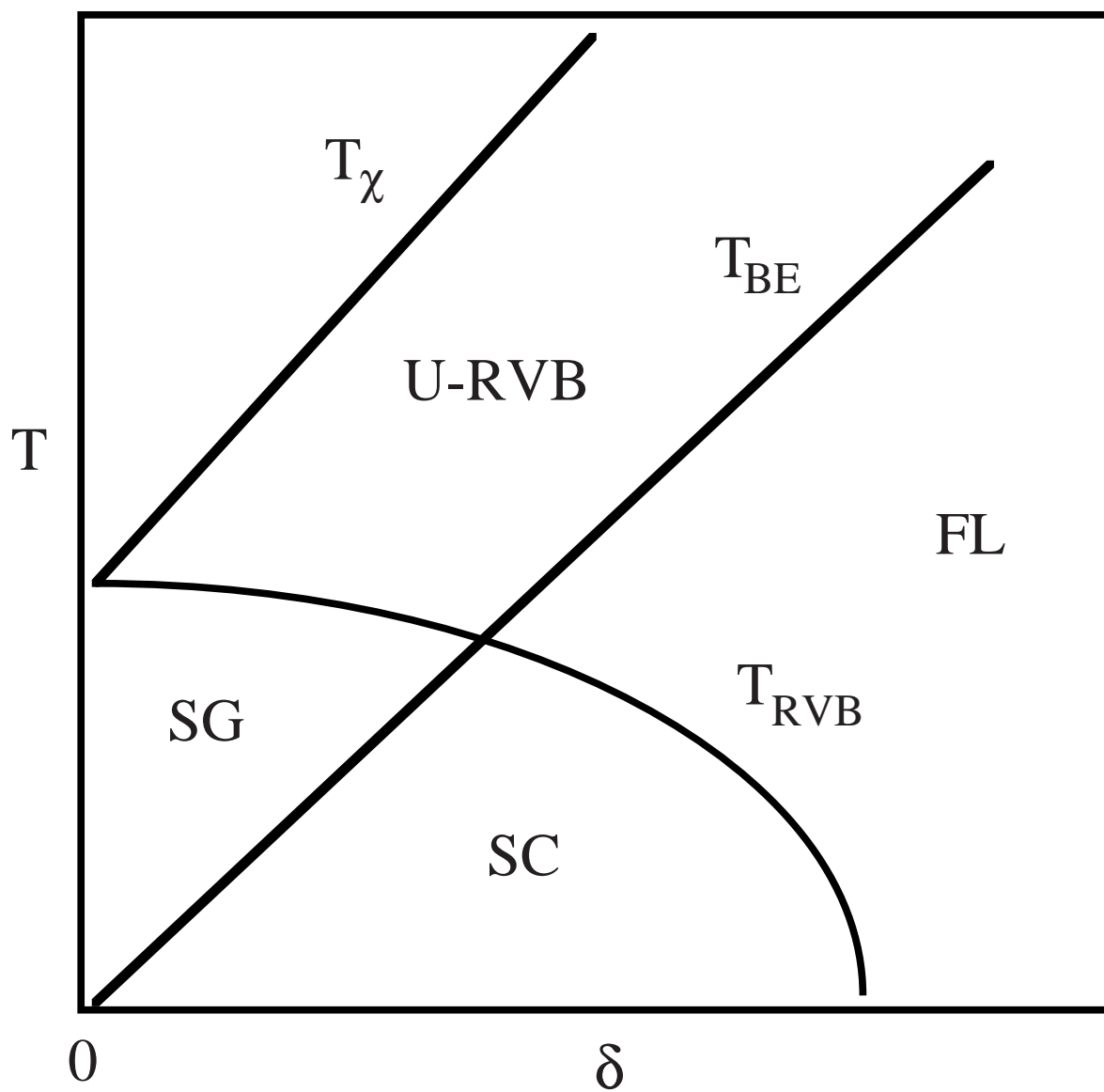


Fig1

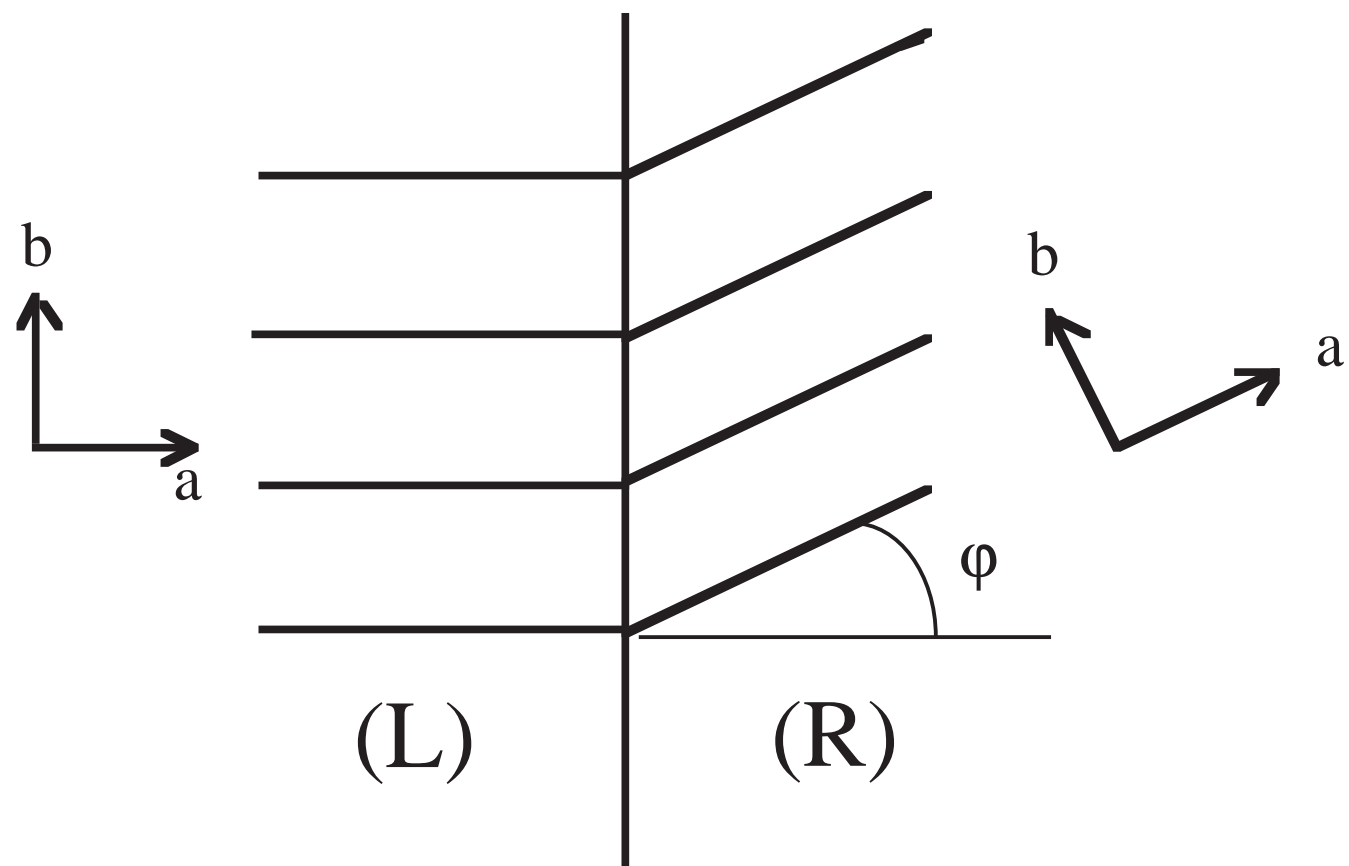


Fig2

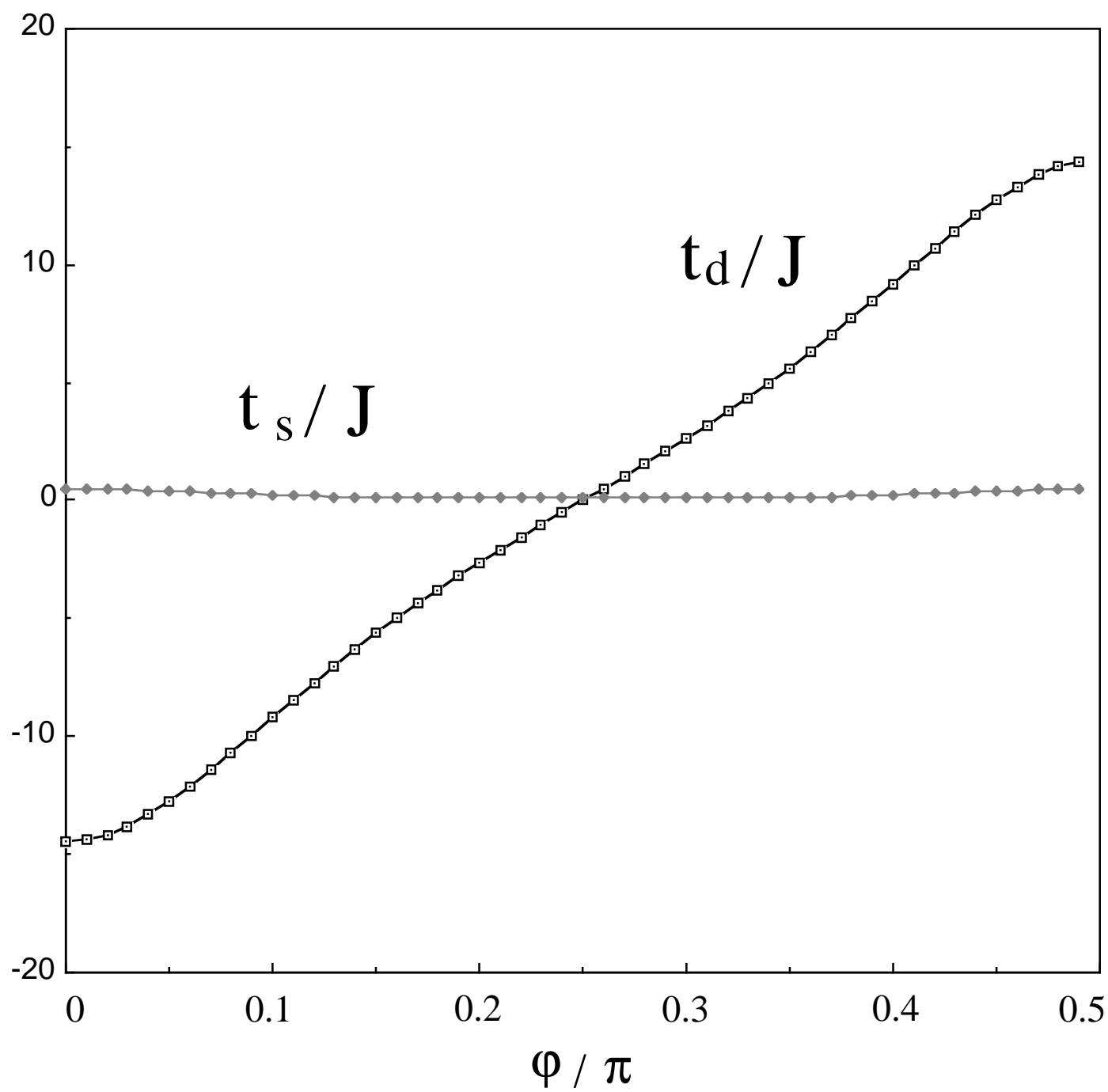


Fig3a

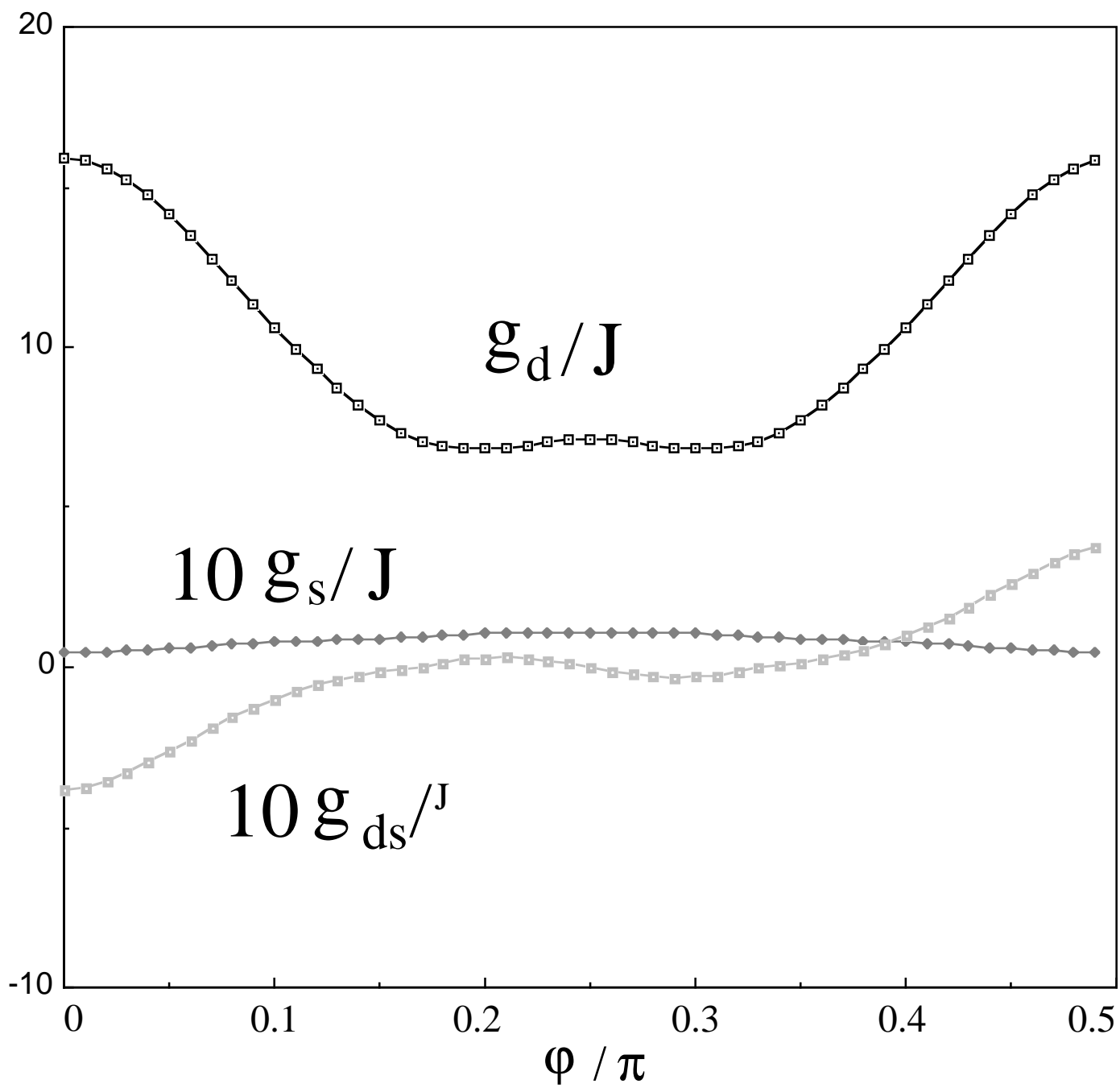


Fig3b

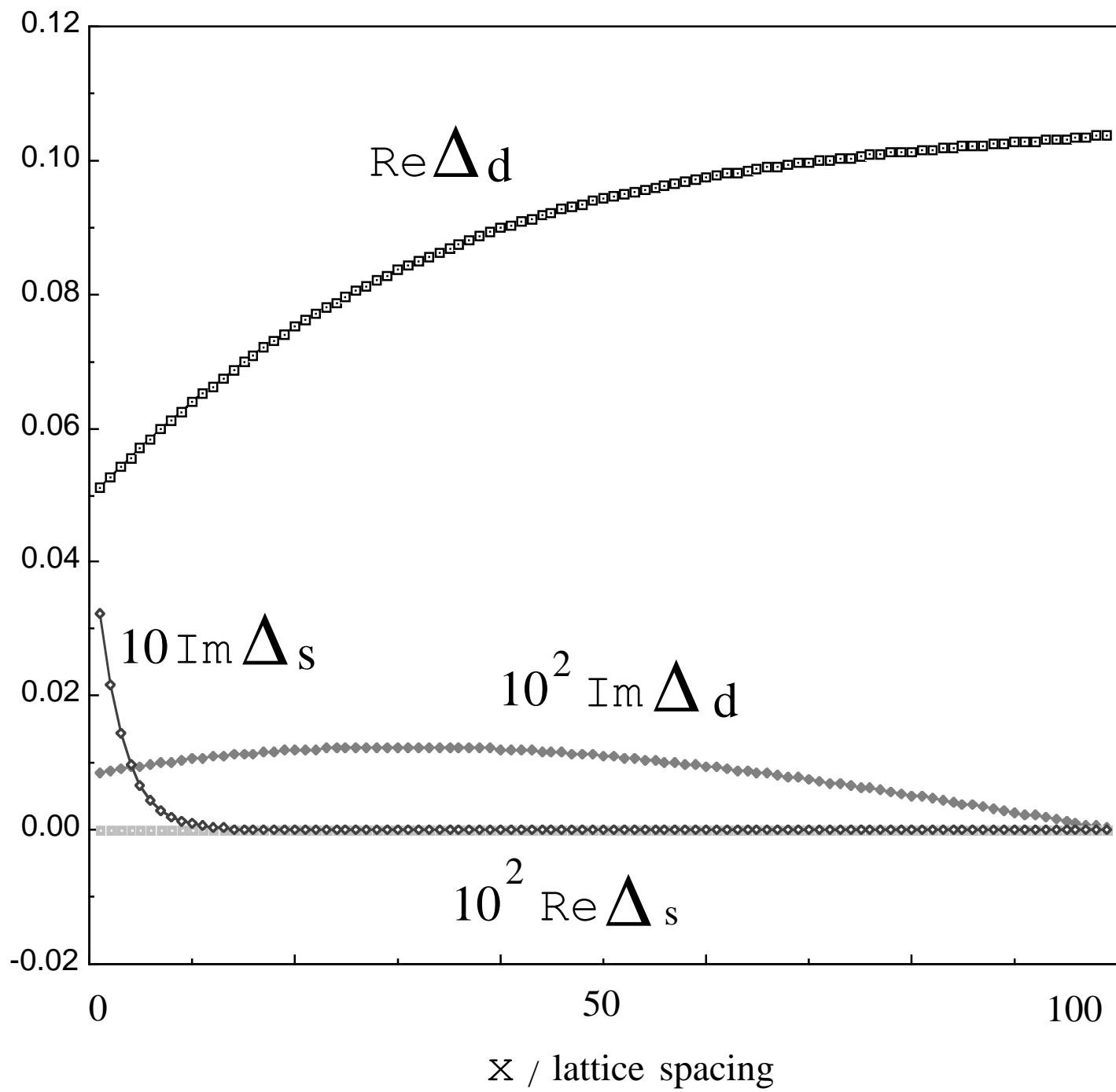


Fig4

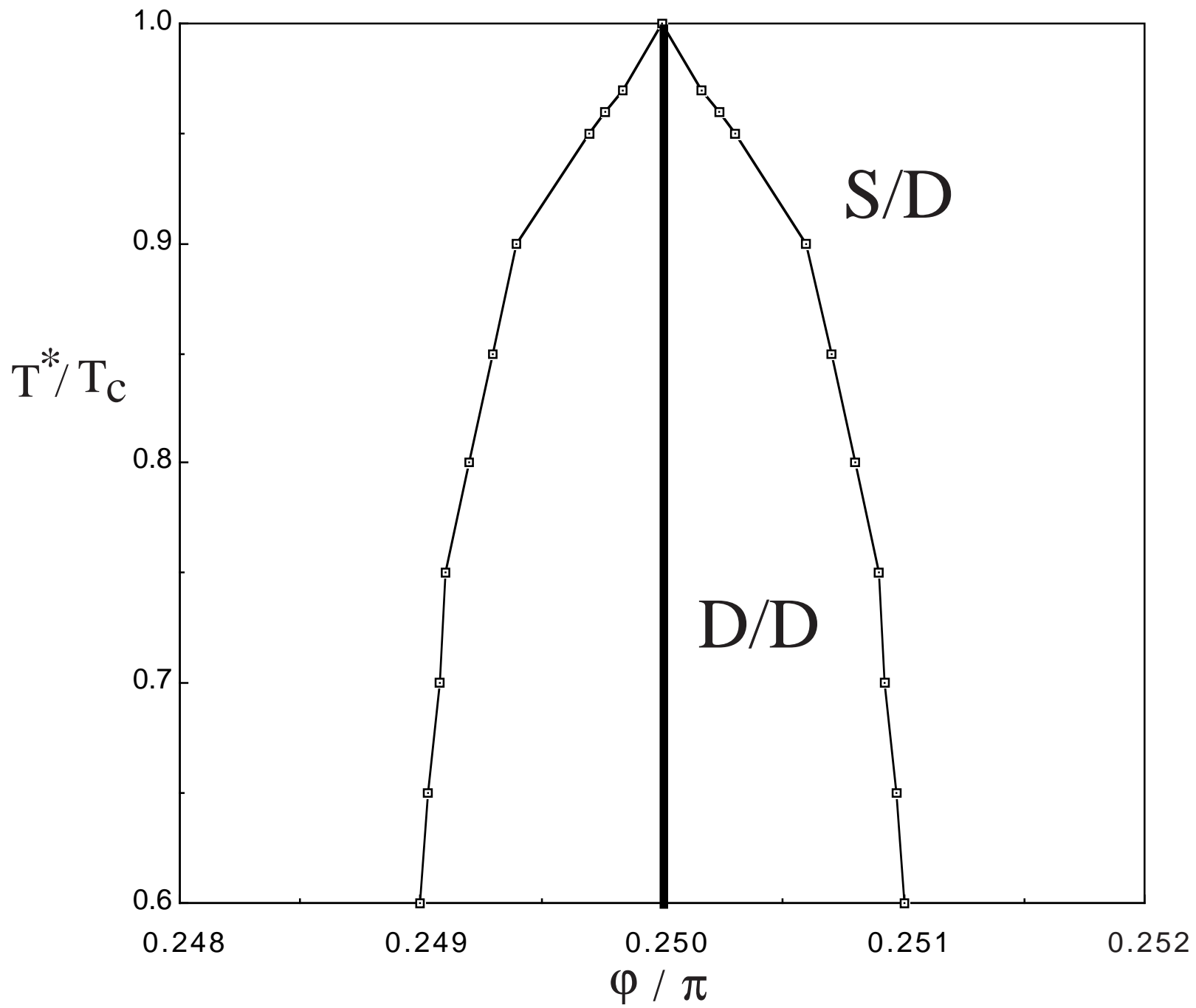


Fig5

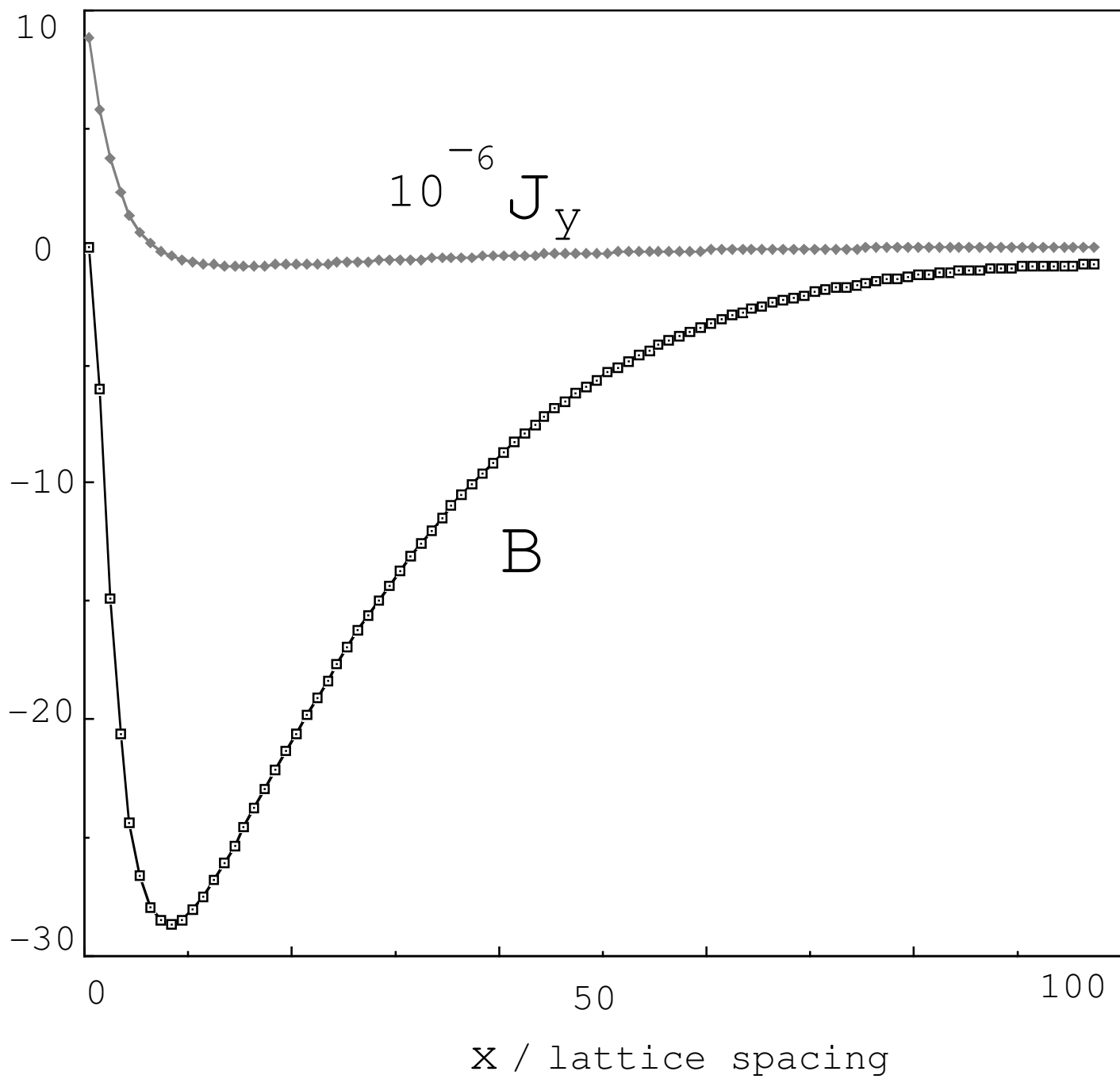


Fig6

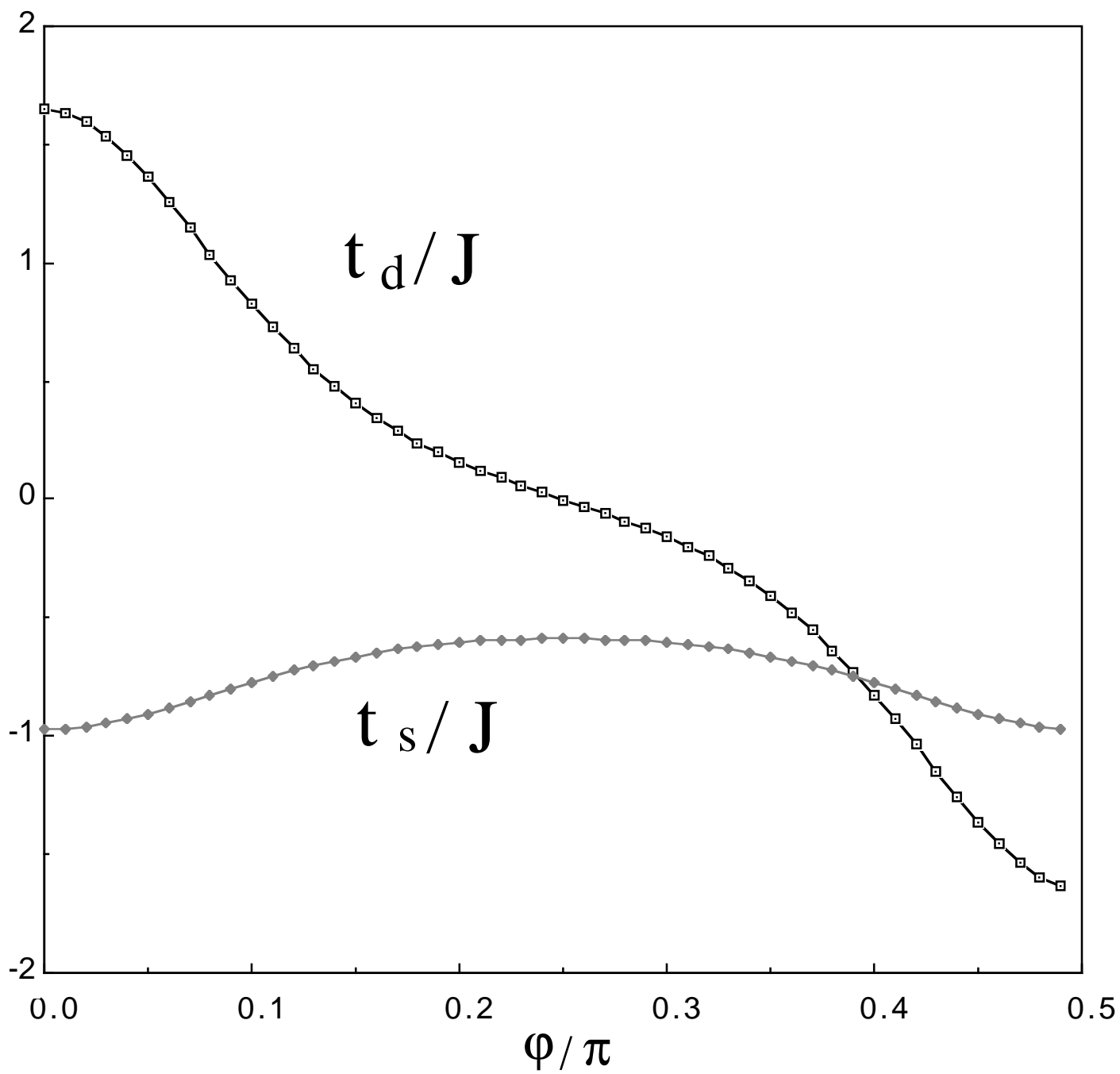


Fig7

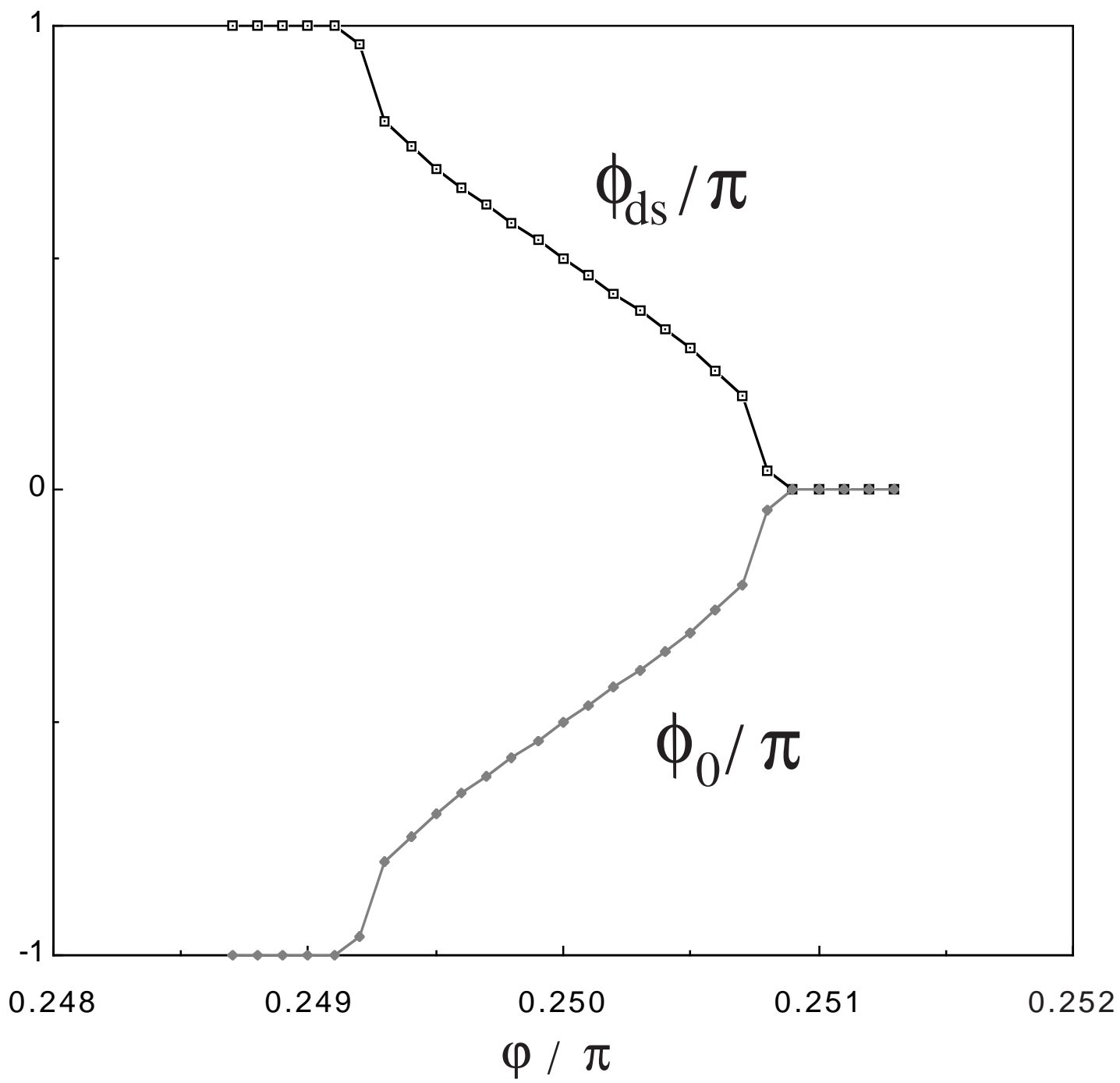


Fig8